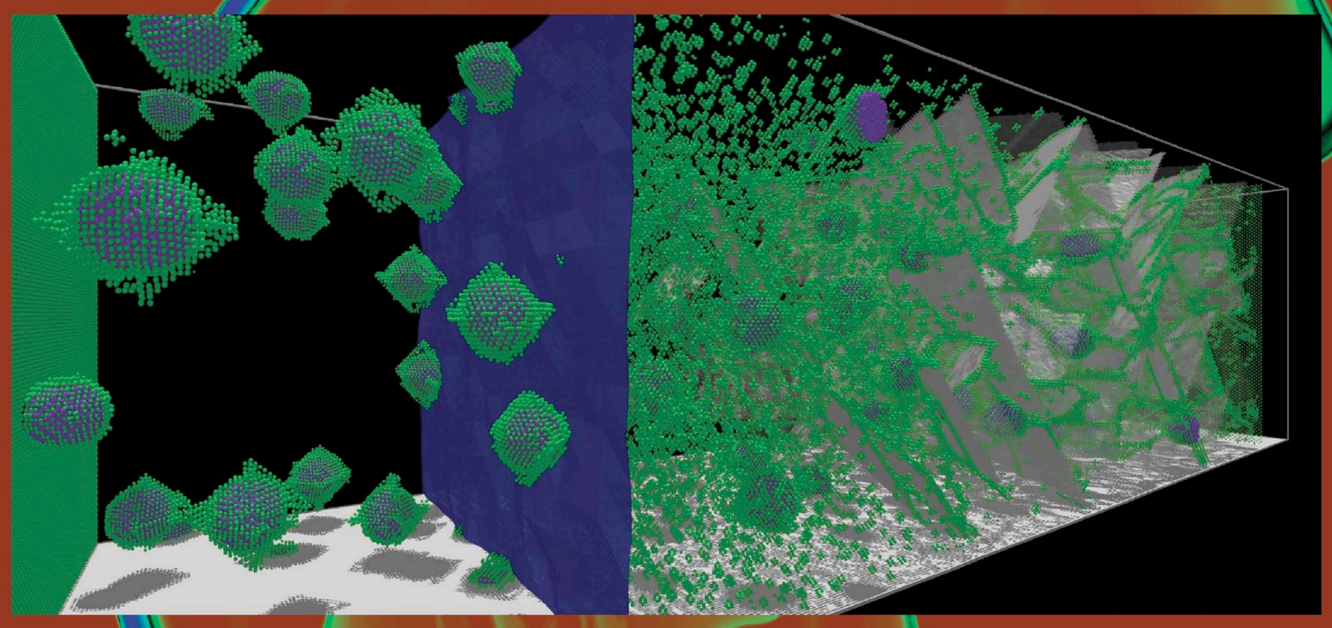
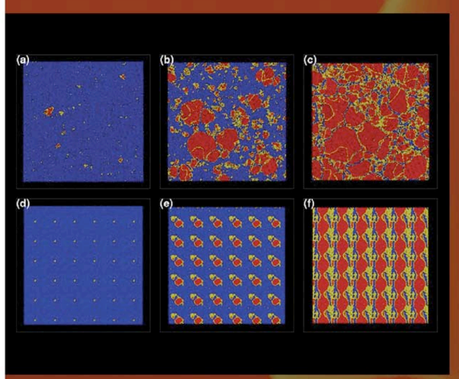
Advancing Science



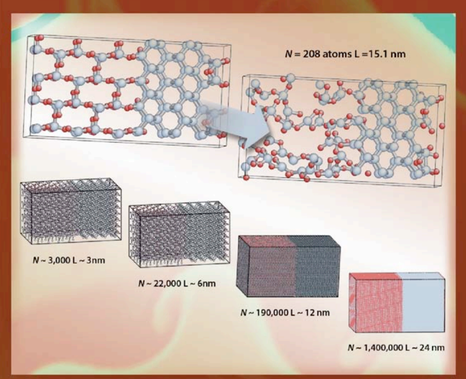
Shock compression at 12 GPa of aluminum with helium bubbles

Advancing Physics Understanding

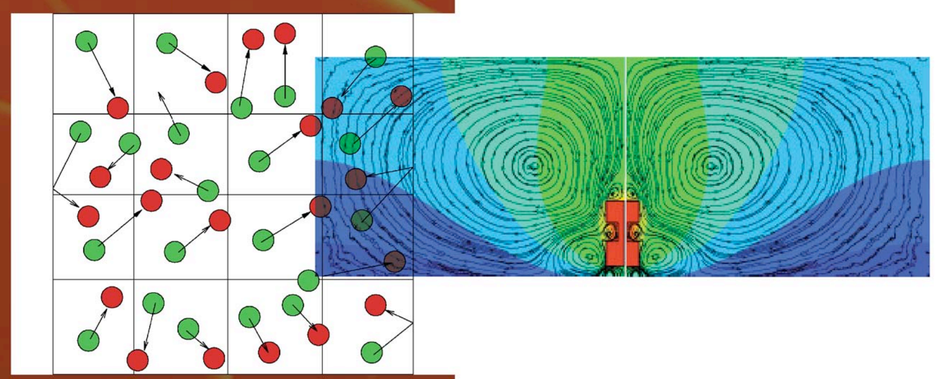
A major ASC theme is to improve predictive capability by investigating key physical phenomena and removing the ad hoc models used to represent physical mechanisms that are not sufficiently understood. Models at the sub-grid scale, and extending to molecular and atomic scales, are needed to understand the critical physics for nuclear weapons simulations. Until recently the codes, computers, and computing infrastructure did not exist to support realistic modeling at the length scales of interest. However, new supercomputing capabilities have made modeling at the atomic and molecular levels possible, and these capabilities produced by the ASC Program are beginning to increase the necessary sophistication with which problems such as plutonium aging can be addressed .



Snapshots from simulations of solidification in tantalum. The top sequence displays nucleation (a) and growth (b) occurring in a 16,372,000-atom simulation, resulting in a realistic distribution of grains and grain boundaries (c). The same process modeled using 64,000 atoms (d–f) produced the artificial final structure shown in (f).



Molecular simulation on ASC computers is being used to study chemical processes in materials . This work has important applications to the aging and reliability of a variety of weapon components (e.g., semiconductors, HE, polymers). The GRASP parallel molecular dynamics code uses the ReaxFF force field to simulate the evolution of positions, bonding, and charge states of large numbers of atoms.



The ASC program is developing physics models for micro-mechanical devices. Direct S imulation Monte-Carlo (DSMC) is a numerical method to describe non-continuum phenomena at these micro-scales.

This visualization shows the results of a DSMC simulation for non-continuum energy transport in a gas driven by temperatures in the absence of buoyancy.

Supercomputing
Conference 2005

Visualize the Difference

National Nuclear Security Administration